

The Arctic Terrestrial Simulator: Modeling Permafrost Degradation in a Warming Arctic

Ethan Coon,
Rao Garimella,
Gianmarco Manzini,
J. David Moulton,
Daniil Svyatskiy, T-5;
Markus Berndt, CCS-2;
Scott Painter, EES-16

The terrestrial Arctic has been a net sink of carbon for thousands of years, but warming trends suggest this may change. Predictive simulation of the fate of this carbon is critical for understanding feedback effects between the terrestrial Arctic and climate change. Toward this end, a flexible, versatile modeling capability called the Arctic Terrestrial Simulator (ATS) is being developed. Here we introduce the modeling challenges of the problem and discuss computational advances required for predictive simulation, including the development of a multiphysics simulation framework and meshing infrastructure.

Researchers at LANL are developing a new high-performance simulation tool—the ATS—to study the effects of climate change on the release of massive amounts of carbon currently frozen in the Arctic.

It is estimated that approximately 1,700 billion metric tons of organic carbon are frozen in the Arctic permafrost [1]. The tipping point for the release of this carbon in the form of greenhouse gases due to permanent degradation of the permafrost is unknown [2]. Degradation of the permafrost, consequent evolution of the topography, the resulting restructuring of the drainage networks, and their effect on the vegetation are poorly understood. Computer modeling is a key tool in untangling these complex couplings to understand the evolution and potential feedback of the Arctic and subarctic landscapes on the global climate system.

LANL researchers are developing ATS as a ground-breaking modeling capability to simulate freeze/thaw cycles in the arctic soil, snow melt and runoff, subsurface flow due to infiltration and ice melt, soil subsidence due to the melting ice, and biogeochemical

is a multi-lab program developing a state-of-the-art approach and open-source integrated toolset for the assessment and management of DOE legacy waste sites. The combined arctic processes in ATS and multiphysics capabilities in Amanzi are called Amanzi-ATS.

Amanzi-ATS is built with flexibility and modularity as its main design principles. Individual problems simulated using Amanzi-ATS may require different processes, or may require coupling different processes in different ways, to correctly capture the essential physics. To accomplish the flexibility required, processes are combined in a tree structure that characterizes how Process Kernels (PK) are coupled (see Fig. 1 for a schematic of a possible PK layout for the full Arctic system). PKs are coupled via multi-process coordinators (MPC), which can encapsulate weak (operator-split) or strong (fully implicit) coupling. At any node in the PK tree, a time-integration scheme and nonlinear solver for the coupled subsystem consisting of all PKs below that node in the tree can be automatically formed and solved. This automated coupling allows complex systems to be built and tested quickly and easily. If needed, special couplers can be written that automate most of the process but allow the inclusion of extra coupling terms for preconditioners or solvers.

This PK tree makes it trivial to include, or exclude, individual processes in a given simulation. This is important for two reasons. First, it makes testing individual processes easier. Tests are built up hierarchically, testing first one process, then two coupled processes, then multiple processes together. This builds confidence in the code. Second, it makes evaluating scientific hypotheses easier. Swapping PKs enables different physics to be included, or excluded, determining whether a given process is important to the question of interest.

Amanzi-ATS also has a sophisticated parallel mesh infrastructure to manage the multiple meshes required and then deform those meshes. These meshes are typically formed from data, including topography,

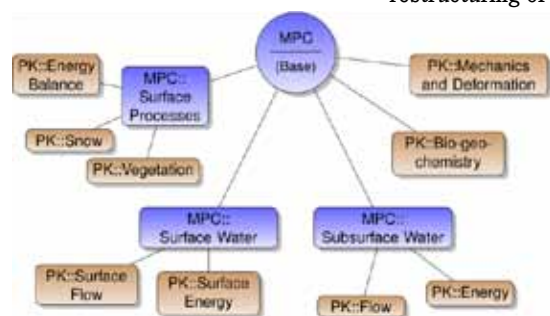


Fig. 1. A schematic of the PKs and coupling needed for permafrost simulation. Brown nodes indicate physical process kernels, which describe one process. Blue nodes MPC, which couple the process kernels below them. To enable the tree structure, MPCs are also themselves PKs, presenting an interface for describing the coupled system as one PK to the MPC above it. The top level (Base) MPC manages the coupling of each subsystem and advances the entire simulation.

processes in the vegetation layer [3]. This is a computationally challenging problem because of the number and complexity of the controlling physical processes, and the strong coupling between these processes. Necessarily fine spatial and temporal resolution, in conjunction with nonlinearities due to the freeze/thaw cycle, pose additional difficulties for the simulator. Finally, handling the evolving topography places demanding constraints on the mesh infrastructure and discretization strategies.

The ATS is based on Amanzi [4], the open-source flow and reactive-transport simulator being developed by the Advanced Simulation Capability for Environmental Management (ASCEM) program. ASCEM

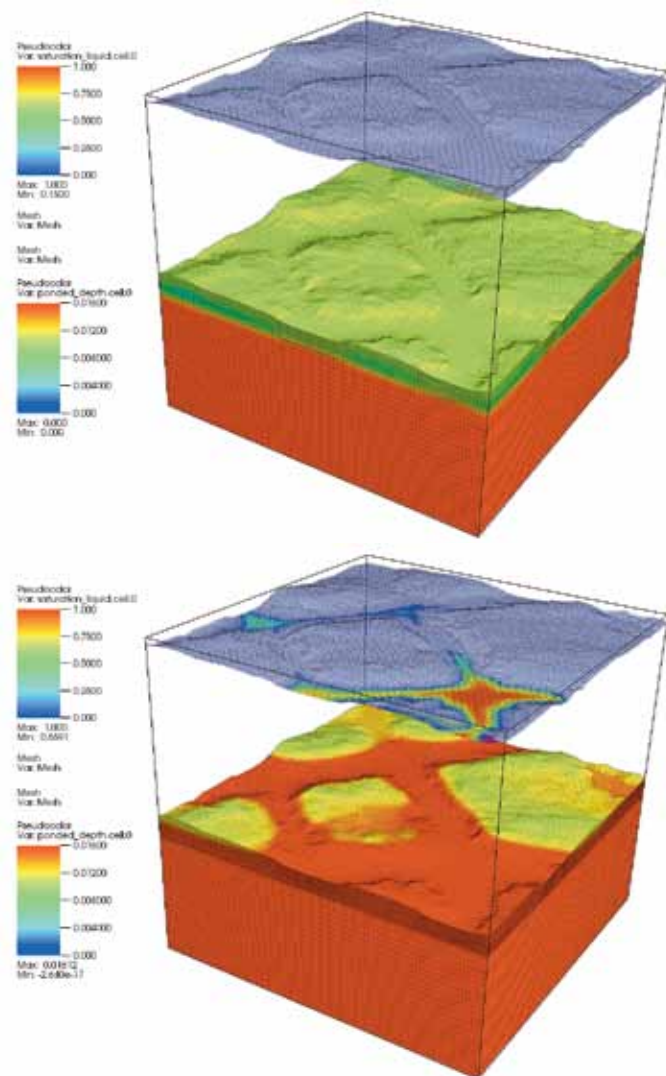


Fig. 2. A demonstration of coupled surface/subsurface flow for high-centered polygons at Barrow, Alaska. In these visualizations, the surface mesh has been raised above the subsurface mesh. Rain falls on the surface of the domain, with initial water table shown (top). The rainfall infiltrates the subsurface until the water table rises above the surface in some regions, where it pools (bottom). The meshes are formed and managed by advanced mesh infrastructure, while coupling is automated by the multiphysics capabilities of Amanzi-ATS.

from sites such as Barrow, Alaska. The mesh infrastructure in Amanzi-ATS wraps the LANL-developed MSTK mesh framework and provides additional functionality tailored specifically for the processes in the Arctic simulations. The process kernels in Amanzi-ATS can query the mesh for entity geometry, topology, and connectivity. In addition, entity sets based on geometrically defined regions are available—these are used for assigning initial conditions, boundary conditions, or material properties. The mesh infrastructure in Amanzi-ATS is capable of reading very large 3D meshes in parallel and weaving them together for the subsurface flow and freeze/thaw simulations. The top surface of the meshes on each partition is extracted and then woven together, forming a parallel surface mesh for overland flow simulation. Finally, Amanzi-ATS also has the ability to deform meshes as driven by a soil subsidence model resulting from ice melt. The subsidence model computes a set of nodal displacements, and the mesh infrastructure attempts to deform the mesh while maintaining the validity of elements.

Amanzi-ATS simulations have been conducted on up to 10,000 processors on LANL institutional clusters. These simulations include the coupled overland and subsurface flow shown in Fig. 2 and cyclic freeze/thaw problems on geological domains in the Arctic.

During the next year, Amanzi-ATS will be developed further to include subsidence, snow, and biogeochemical processes, and to couple these processes. These advances will test both the multi-physics framework and the mesh infrastructure highlighted here. As this predictive simulation capability matures, it will be used to study realistic what-if scenarios of permafrost degradation and greenhouse gas release.

- [1] Tarnocai, C. et al., *Global Biogeochem Cy* **23**, GB2023 (2009).
- [2] “Climate Change 2007: Synthesis Report,” *Fourth Assessment Report of the Intergovernmental Panel on Climate Change*, **104** IPCC (2007).
- [3] Painter, S. et al., “Modeling Challenges for Predicting Hydrologic Response to Degrading Permafrost,” *Hydrogeology J*, in press (2012).
- [4] Moulton, J.D. et al., “Amanzi et al., the Multi-Process High Performance Computing Simulator,” LANL Technical Report LA-UR 12-22193; ASCEM-HPC-2011-03-1 (2012).